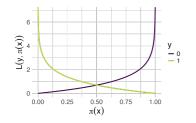
Introduction to Machine Learning

Advanced Risk Minimization Proper Scoring Rules





Learning goals

- Scoring rules on prob. predictions
- First order condition of SRs
- Log loss and Brier are strictly proper
- L1 on probs is not
- 0/1 is proper but not strict

PROB. PREDS / SCORING RULES • Gneiting and Raftery 2007

- Is specific loss $L(y, \pi(\mathbf{x}))$ on a prob. classifier "reasonable"?
- Assume binary classification with $y \in \{0, 1\}$
- Loss can already be called scoring rule, but we also now take expectation over y
- Scoring rule compares predictive vs. label distrib:

$$S(Q, P) = \mathbb{E}_{y \sim Q}[L(Q, P)]$$

- Simply expected loss, now we write P for $\pi(\mathbf{x})$
- We have looked at this before
- As we have seen in the beginning of this chapter: Can do this unconditionally or conditionally, all the same anyway
- Minimizing the above asks then for the risk minimizer!



PROPER SCORING RULE • Gneiting and Raftery 2007

• SR is **proper** if true label distrib Q is among the optimal solutions, when we maximize S(Q, P) in the 2nd argument (for a given Q)

$$S(Q,Q) \leq S(Q,P)$$
 for all P,Q

• Translation (now for conditional): $\mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$ is **among the solutions** for the RM:

$$\eta(\tilde{\mathbf{x}}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}}) \in \pi^*(\tilde{\mathbf{x}})$$

- NB: We were never precise before that the RM as "argmin" is a set!
- S is **strictly proper** when equality holds iff P = Q
- Translation (now for conditional): $\mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$ is unique RM!

$$\pi^*(\tilde{\mathbf{x}}) = \eta(\tilde{\mathbf{x}}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$$

• (Strictly) proper SR ensure optimization pushes solution $\pi(\mathbf{x})$ to Q



L1 LOSS IS NOT PROPER

- Let's look at it unconditionally, so we don't always have to write x
- Binary targets $y \sim \text{Bern}(\eta)$
- For any binary prob. loss *L*:

$$\mathbb{E}_{y}[L(y,\pi)] = \eta \cdot L(1,\pi) + (1-\eta) \cdot L(0,\pi)$$

• Let's check L1 loss $L(y, \pi) = |y - \pi|$

$$\mathbb{E}_{y}[L(y,\pi)] = \eta |1 - \pi| + (1 - \eta)\pi = \eta + \pi(1 - 2\eta)$$

- Linear in π , but with box constraints
- For $\eta > 0.5$: $\pi^* = 1$
- For $\eta < 0.5$: $\pi^* = 0$
- So π^* usually not the same as η
- True η is worse than RM π^* , so L1 not proper SR



0/1 LOSS IS PROPER – BUT NOT STRICT

- ullet 0/1 loss $L(y,\pi)=\mathbb{1}_{\{y
 eq h_\pi\}}$ using hard labeler $h_\pi=\mathbb{1}_{\{\pi\geq 0.5\}}$
- Expected loss:

$$\mathbb{E}_{y}[(y,\pi)] = \eta \cdot L(1,\pi) + (1-\eta) \cdot L(0,\pi)$$

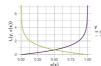
$$= \begin{cases} \eta & \text{if } h_{\pi} = 0 \\ 1-\eta & \text{if } h_{\pi} = 1 \end{cases}$$

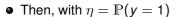
- So expected loss only takes 2 values
- For $\eta \geq 0.5$, minimal if $h_{\pi} = 1$ \rightarrow any $\pi \in [0.5, 1]$ minimizes
- For $\eta <$ 0.5 expected loss is minimal if $h_{\pi} =$ 0 \rightarrow any $\pi \in [0, 0.5)$ minimizes
- True η among solutions \rightarrow proper
- True η is not unique minimizer \rightarrow not strictly proper



DISCOVER PROPER SCORING RULES

- How define L such that $\mathbb{E}_y[L(y,\pi)]$ is minimized at $\pi^* = \eta$?
- Assume symmetry: $L(1,\pi) = L(\pi)$ and $L(0,\pi) = L(1-\pi)$
- Remember that when we plotted such losses, we usually had 2 curves, symmetric at $\pi=0.5$?





$$\mathbb{E}_{\mathbf{y}}[L(\mathbf{y},\pi)] = \eta \cdot L(\pi) + (1-\eta) \cdot L(1-\pi)$$

• First-order condition: Set $L'(\pi) = 0$, and $\pi = \eta$ at minimum

$$\eta \cdot L'(\eta) \stackrel{!}{=} (1 - \eta) \cdot L'(1 - \eta)$$



LOG LOSS / BRIER ARE STRICTLY PROPER

• First-order condition:

$$\eta \cdot L'(\eta) \stackrel{!}{=} (1 - \eta) \cdot L'(1 - \eta)$$

- One solution is $L'(\eta) = -1/\eta$
- Antiderivative is $L(\eta) = -\log(\eta)$
- Remember: $L(1,\pi) = L(\pi)$ and $L(0,\pi) = L(1-\pi)$
- This is log loss

$$L(y,\pi) = -y \cdot \log(\pi) - (1-y) \cdot \log(1-\pi)$$

- Second solution is $L'(\eta) = -2(1 \eta)$
- Antiderivative $L(\eta) = (1 \eta)^2$
- So Brier score

$$L(y,\pi)=(y-\pi)^2$$

• Both strictly proper (check 2nd derivative for strict convexity)



OUTLOOK

- Usually SRs are maximimized, I adapted notation a bit here for us, to get a direct connection ERM
- Was easier to talk about binary classification here, but proper SRs are defined in general
- There are other proper SRs, like "generalized entropy score" or "continuous ranked probability score"
- We only scratched surface of theory
- If you want to know more: start by reading the Gneiting paper

